AEC Computing Facility

PHYSICS AND
MATHEMATICS

NYO-7976

A MONTE CARLO CALCULATION
OF THERMAL UTILIZATION

by

A. Rotenberg, A. Lapidus and
R. D. Richtmyer

January 15, 1958

institute of mathematical sciences

NEW YORK UNIVERSITY

NEW YORK, NEW YORK

AEC Computing and Applied Mathematics Center
Institute of Mathematical Sciences
New York University

PHYSICS AND   NYO-7976
MATHEMATICS

A MONTE CARLO CALCULATION
OF THERMAL UTILIZATION

by

A. Rotenberg, A. Lapidus and
R. D. Richtmyer

January 15, 1958

ABSTRACT

A Monte Carlo program to evaluate the thermal utilization of neutrons in a water moderated lattice reactor with slightly enriched uranium fuel rods has been written for UNIVAC. Histories were started off assuming that neutrons enter the thermal region as a result of a hydrogen collision at high energy (> 3 e.v.) and each neutron was given unit weight. At each collision the weight factor was reduced by a factor $\Sigma_a/(\Sigma_a + \Sigma_s)$. Histories were terminated by a Russian roulette technique. Other methods of termination were tried but this one was by far the most efficient. The water was treated as a monatomic hydrogen gas having a constant scattering cross-section of 20 barns and having the density of hydrogen in liquid water. A 1/v law was assumed for all absorptions, except in the case of U-235 where an empirical formula was used to fit the data given in BNL-325. At collisions in moderator a rejection procedure was used to choose protons from a Maxwell-Boltzmann distribution. Comparison of the results with those obtained experimentally at Westinghouse (Bettis) and Brookhaven showed agreement to within 1 % for

several different sizes of fuel rods and water to
uranium ratios. This is better than was expected
considering the approximations made. A new version
of the code, which will take into account the effects
of inelastic scatterings by using a quantum mechanical
isotropic oscillator model of the water molecule, is
being written for the IBM-704.

TABLE OF CONTENTS

A MONTE CARLO CALCULATION OF THERMAL UTILIZATION

1. Introduction

As a part of the continuing study of the feasibility of performing reactor calculations by Monte Carlo methods a UNIVAC code has been written to calculate the thermal utilization factor. The reactors chosen for this investigation were very similar to experimental reactors [1] for which data are known. These reactors have slightly enriched uranium fuel rods in a lattice arrangement and use ordinary water as moderator.

In this code, neutron histories are simulated, with certain approximations which are discussed in detail below, beginning at some "high" energy E_{MAX} and continuing until absorption takes place. A "high" energy is defined as one much above the thermal region but well below the lowest resonance in the fuel. Thermal utilization, as measured by the code, is defined as the ratio

$$f = \frac{\text{Number of neutrons captured in fuel}}{\text{Total number of neutrons captured}} \qquad (1)$$

where capture includes fission and all processes such as (n,γ), (n,p) and (n,α) by which neutrons are absorbed.

In this report, the reactor model used is described

in Section 2. In Section 3 the method used to handle scatterings of neutrons in the water is presented. The Monte Carlo sampling techniques used to estimate the thermal utilization follow in Section 4. Some results of the calculations are given in the following section and finally there is a description of new work in progress.

2. The Reactor Model

In order to have some criterion for judging the accuracy of the results, a model was chosen to approximate the experimental reactors [1] at Westinghouse (Bettis) and Brookhaven for which thermal utilization measurements have been made. These reactors have slightly enriched uranium rods in aluminum cans in a hexagonal lattice arrangement in a moderator of ordinary water. For simplicity, a square rather than a hexagonal array was used in the code. The extra computing time required to perform the calculation for hexagonal lattices would not have been very long but neutrons in the lattices have a tendency to remain in the cell where they are born and so the different lattice arrangement affects the thermal utilization only slightly.

The code assumes that the array extends infinitely in every direction. However, all neutrons are considered to remain inside one lattice cell (see Figure 1, page 9). If a neutron leaves this cell as at 1A or 2A in the figure, a transformation is made to bring it back into the basic cell at 1B or 2B, and at the same time a record is kept that the neutron has moved one cell in the appropriate (positive or negative) x or y direction. There are no restrictions in the code

on travel in the z-direction.

In the experimental reactors there is a thin air gap between the uranium rods and the aluminum cladding. In the code the whole space taken up by the air and the aluminum (region 1 in Figure 1) is considered to be vacuum since the cross-sections are small. Thus, in the code, only collisions in moderator and fuel are considered.

Neutron histories are started off assuming that neutrons first enter the region below E_{MAX} as a result of a collision with a hydrogen atom at an energy above E_{MAX} and these neutrons are assumed to be uniformly distributed in energy from E_{MAX} down to zero. It follows that neutron histories begin only in the moderator. It is further assumed that the starting distribution is uniform in the moderator, and that the starting velocities are spherically symmetric. These assumptions are good only for a fuel like uranium where the lowest resonance at 6.7 e.v. is well above thermal energies; for a fuel having resonances down into the thermal region, resonance escape and thermal utilization would not be clearly separated and this picture would be invalid. The maximum energy E_{MAX} given to neutrons by the code is chosen to be 3 e.v.
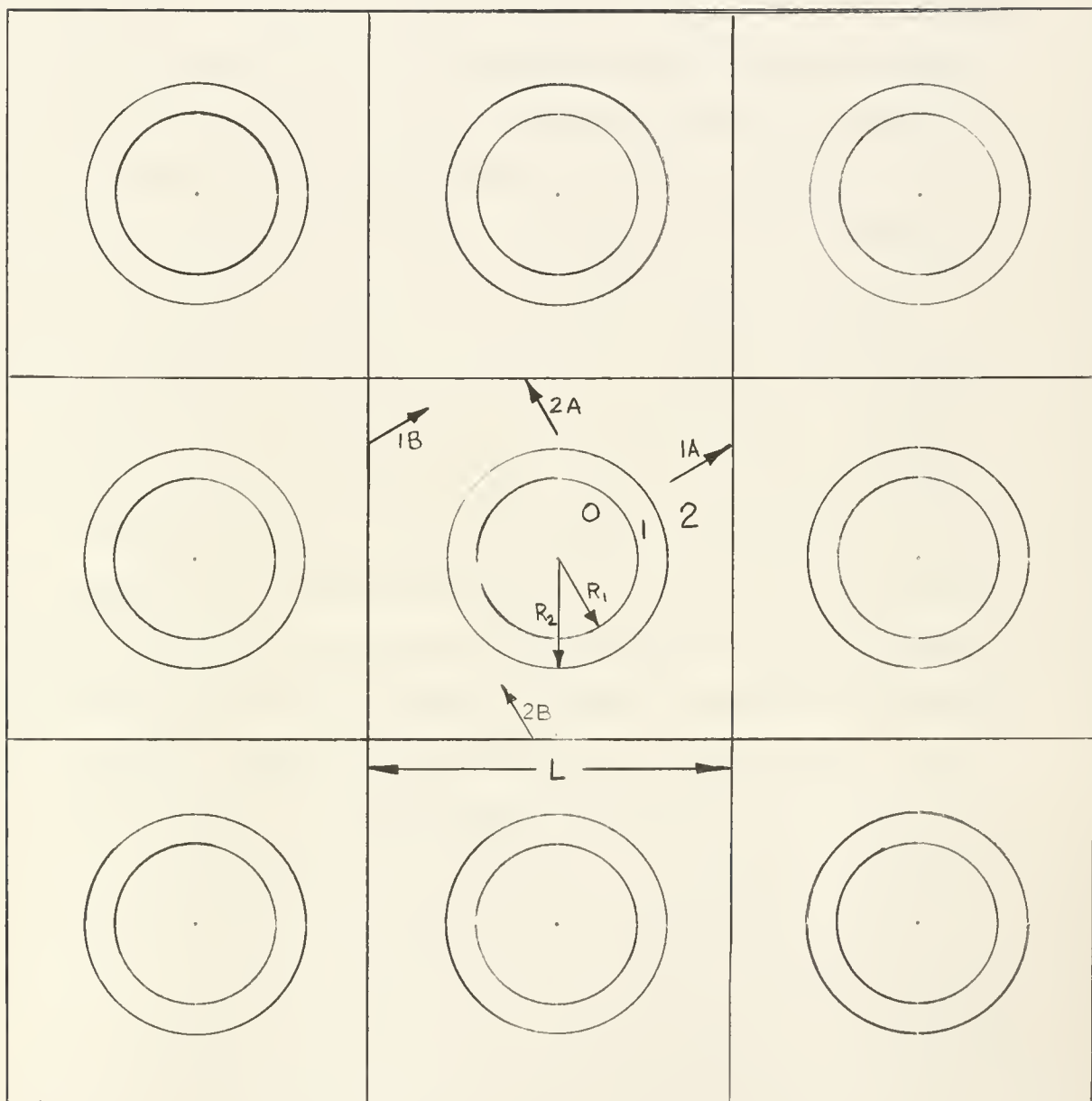
Figure 1.   The Lattice Arrangement.   Region O is fuel, 1 vacuum,
and 2 moderator.   Arrows 1A, 1B and 2A, 2B indicate how
transformations are made so that all neutrons remain in
the basic cell.

In accordance with these assumptions a neutron history begins at some point (x,y) in the lattice, with the neutron travelling with a velocity $\vec{v}$. To choose the coordinates uniformly and randomly in the moderator, two random numbers ξ_1 and ξ_2 are chosen in the interval $(-1,1)$. These numbers are multiplied by $L/2$ (where L is the length of one lattice square, see Figure 1) and assigned to x and y respectively. If $x^2 + y^2 > R_2^2$ where R_2 is the outer radius of the cladding, these coordinates are accepted, otherwise new random numbers are chosen until a pair is found satisfying the inequality. The speed is chosen by taking a random number in $(0,1)$ and multiplying it by v_{MAX}, the velocity corresponding to an energy of 3 e.v. The direction angles θ and ϕ can be obtained by choosing a random number in $(-1,1)$ and setting it equal to $\cos \theta$, and another random number in $(0,2\pi)$ and setting it equal to ϕ. Since the cosine and sine of both angles are desired this procedure requires the calculation of $\cos \phi$ and two square roots must be extracted to obtain the sines. A method of obtaining the sines and cosines with the appropriate distributions due to von Neumann [2] and requiring only one square root is used since it is much faster. Once the position and velocity of the neutron are known it is a matter of

simple analytic geometry to calculate how far the neutron
will travel before reaching a boundary. A boundary can
be either the imaginary square which defines the lattice
or else the surface of another region. In the actual
lattices, the only region a neutron can enter from the
moderator is that of the aluminum cladding around the
uranium fuel rod, region 1 in Figure 1. Now it must
be determined whether the neutron will reach the
boundary or whether it will suffer a collision before
doing so. If $\sum$ is the total macroscopic cross-
section, then the probability that the neutron will
travel a distance s and undergo a collision in s+ds
is $e^{-\sum s}$. Thus the distance s must be chosen from
an exponential distribution and this is done by taking
the negative of the logarithm of a random number chosen
on (0,1) and setting it equal to η. Then
$\eta \sin \theta / \sum$ is the distance s, since the projection
of the actual distance on the x-y plane will deter-
mine where the next collision occurs in that plane.
If s is greater than the distance d to the boundary,
the neutron is moved to the boundary point and a new s
and d are found. If a cell boundary is reached, the
appropriate reflections are effected as already
described. In the case where a new medium is entered
the appropriate cross-section must be used in calculating

s, the distance to the next collision. If a collision occurs before the boundary is encountered it is necessary to find out whether this collision is an absorption or a scattering. This is done by a Monte Carlo game of chance as follows: a random number ξ is chosen in the interval $(0,1)$. If $\xi < \sum_a / (\sum_a + \sum_s)$ absorption is decreed to have occured and the history is terminated. Otherwise the collision is deemed a scattering one, and the neutron emerges from the collision with a new velocity and direction. A full description of the treatment of neutron collisions in hydrogen is given in the next section where it is shown how the velocity after a hydrogen collision is obtained. The only heavy scatterer taken into account by the code is uranium which is assumed to be infinitely heavy so that neutron scatterings by U are spherically symmetric in the laboratory system.

After each non-absorbing collision a new s and d are chosen as before and the calculation continues until an absorption finally takes place. The region where the absorption takes place is recorded and the ratio of absorption in fuel to total absorptions is our estimate of thermal utilization. In Section 4 other sampling procedures which give better estimates of the thermal utilization factor are discussed.

3. Scattering in Hydrogen

The biggest difficulty is calculating thermal utilization whether by transport theory, or by Monte Carlo, is that the velocity distribution of the moderator atoms is not known. For a moderator consisting of a monatomic gas a Maxwell-Boltzmann distribution could be used. However, actual moderators have molecular or crystal structure (or both) to complicate the velocity distributions. Furthermore these structures give rise to the possibility of inelastic collisions which are difficult to handle not only because the processes themselves are very complicated, but in some cases they are imperfectly understood.

In water, the hydrogen atoms are bound to the oxygen in such a way that both rotational and vibrational modes of excitation are possible. There is the further complication in the liquid phase that some of the rotations are hindered because of the interactions of neighboring molecules. It is thus evident that some simplifying assumptions have to be made in order to treat collisions of neutrons with water molecules. For a preliminary study the assumptions are made that the moderator consists only of hydrogen atoms; that these atoms have a Maxwell-Boltzmann distribution of velocities; that the hydrogen scattering cross-section

is constant over the whole thermal range and that these
hydrogen atoms have a density equal to the density of
hydrogen atoms in water at room temperature. Thus
neutrons are assumed to collide with individual atoms,
not with molecules or crystals. These assumptions are
probably invalid for water but nevertheless may be
expected to give a qualitative picture of thermal
utilization. For a graphite moderated reactor the
cyrstal effects are at energies much below thermal and
so the assumption of atomic collisions may be better
than for water. Although these assumptions are admit-
tedly simplifying in the extreme, it is not unreasonable
to expect them to give at least a fair estimate of thermal
utilization. In a homogeneous reactor, consisting of a
fuel and moderator only, the definition of thermal utili-
zation can be written

$$f = \frac{\sum_F^{ABS}}{\sum_F^{ABS} + \sum_M^{ABS}} \tag{2}$$

where $\sum_F^{ABS}$ and $\sum_M^{ABS}$ are the macroscopic absorption
cross-sections, averaged over energy, in fuel and moder-
ator respectively. Since this expression does not depend
upon the scattering cross-sections at all it is reason-
able to assume that for lumped fuel reactors the thermal
utilization will not depend very strongly on the

scattering cross-sections. This is expected to be a better assumption for water moderated reactors than for graphite moderated ones where the fuel rods are much farther apart.

Scatterings in hydrogen involve two problems, choosing a velocity from the Maxwell-Boltzmann distribution of velocities and accounting for the asymmetry in the distribution of protons undergoing collisions. The latter problem can be illustrated by the trivial case where neutron and hydrogen atoms are travelling with the same speed. If both particles are travelling in the same direction they will never collide whereas if they are travelling in opposite directions there is a finite probability of a collision. This is clear from the expression derived below for the scattering rate. Let v, θ, ϕ specify the velocity (speed and direction in spherical polar coordinates with respect to the z-axis which is along the center of the infinitely long fuel rod) of the neutron of mass M before impact and let v_1, θ_1, ϕ_1 specify the same afterwards. Next the scattering rate must be determined for a neutron travelling the speed v in a moderator consisting of atoms of mass AM. Let $N^A(V_x, V_y, V_z) dV_x dV_y dV_z \equiv N^A(\vec{V}) d^3\vec{V}$ be the number of atoms per unit volume of coordinate space

having velocities in the range $\vec{V}$ and $\vec{V} + d\vec{V}$.
Assuming a Maxwellian velocity distribution, we have
at temperature T,

$$N^A(\vec{V}) = N_0^A \left(\frac{AM}{2\pi kT}\right)^{3/2} e^{-AMV^2/2kT} \tag{3}$$

where N_0^A is the number density of moderator atoms
and k is the Boltzmann constant. Let σ_s^A be the
probability of a scattering collision per unit length
of path for one scattering atom per unit volume, so
that the scattering rate by atoms with velocity $\vec{V}$
is $N^A \sigma_s^A |\vec{V} - \vec{v}|$ per unit time. Here σ_s^A is assumed
to be independent of velocity. Then the total scatter-
ing rate R for a neutron having velocity $\vec{v}$ with
the moderator atoms is obtained by integrating over all
velocities of the moderator atoms. Thus we get

$$R = \sigma_s^A N_o^A \left(\frac{AM}{2\pi kT}\right)^{3/2} \int_0^\infty V^2 \, dV \times$$

$$2\pi \int_0^\pi \sin \textcircled{H} \, d\textcircled{H} \sqrt{v^2 + V^2 - 2vV \cos \textcircled{H}} \; e^{-\frac{AMV^2}{2kT}} \tag{4}$$

$$= \sigma_s^A N_0^A v \, \phi \left(\sqrt{\frac{AM}{2kT}} \, v\right)$$

where we have set $d^3\vec{V} = V^2 \, dV \sin \textcircled{H} \, d\textcircled{H} \, d\phi$ and

$$\phi(u) = \frac{4}{3\sqrt{\pi}} \left\{ \int_0^u (y^3 + 3yu^2) + \int_u^\infty (u^3 + 3uy^2) \right\} \frac{e^{-y^2}}{u^2} \, y \, dy \tag{5}$$

This result was obtained by Wigner and Wilkins [3] and

follows directly by making the indicated substitutions and carrying out the integration over ⒣ in a straightforward manner.

A graph of $\phi(u)$ (see Figure 2) shows that $\phi(u) \longrightarrow 1$ as $u \longrightarrow \infty$, i.e. for large v the motions of the scattering atoms can be ignored and this is true for small V (small T or large A) also. Thus for other than hydrogen scattering, it is a good approximation to ignore the effect of the motions of the scatterers and so for all scatterers other than hydrogen the scattering rate is simply $\sigma_s N_0^A v$.
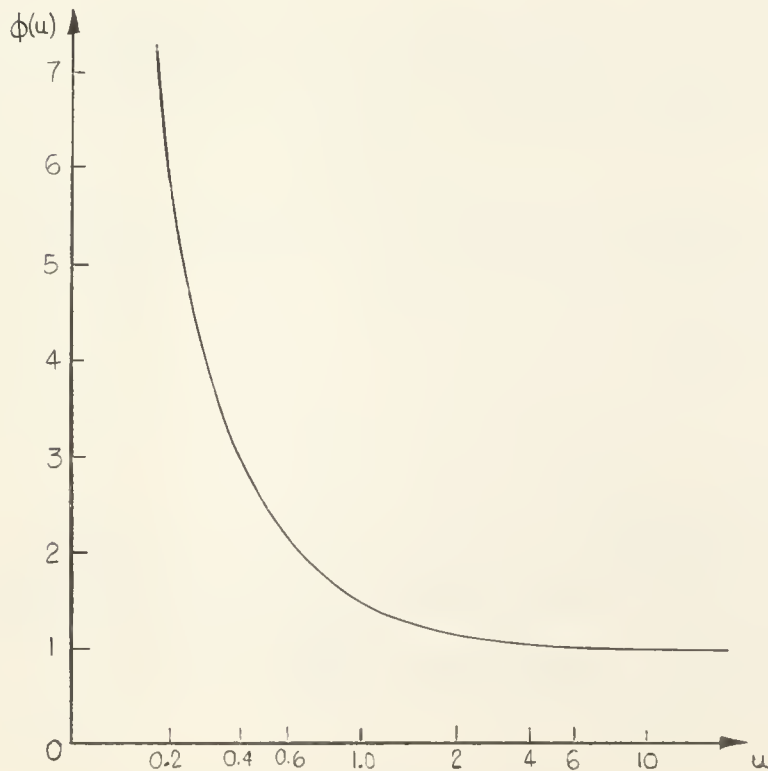

Figure 2

For hydrogen A = 1 and the distribution from which we must choose is

$$p(V,\theta|v) = (\frac{M}{2\pi kT})^{3/2} \frac{\sqrt{V^2+v^2-2Vv\cos\theta}\ e^{-MV^2/2kT}}{v\phi(\sqrt{\frac{M}{2kT}}\,v)} \qquad (6)$$

where $p(V,\theta|v)$ is the probability that a neutron with velocity v has a collision (assuming that a scattering collision does take place) with a molecule having mass M and having a velocity between V and V + dV and that the angle of scattering is between θ and θ + dθ. The procedure used in making a statistically correct choice of V and θ is to take another probability distribution proportional to $g_1(V,\theta|v)$ where

$$g_1(V,\theta|v) = \frac{(\frac{M}{2\pi kT})^{3/2}\ (V+v)\ e^{-MV^2/2kT}}{v\phi(\sqrt{\frac{M}{2kT}}\,v)}\ . \qquad (7)$$

$p(V,\theta|v)$ is a true probability distribution and its integral over all space is unity. It is clear by inspection that

$$g_1(V,\theta|v) \geq p(V,\theta|v) \qquad (8)$$

and if the denominator on the right hand side of equation (7) is decreased the inequality will still hold. Making the substitution $\sqrt{\frac{M}{2kT}}\,V = U$ and $\sqrt{\frac{M}{2kT}}\,v = u$ we get

$$g_1(V,\theta|v)V^2 dV \, d(\cos\theta)d\phi = \frac{(U+u)e^{-U^2}}{(\pi)^{3/2}u\phi(u)} U^2 dU d(\cos\theta)d\phi \quad (9)$$

where the z-axis is taken along the direction of v.

$u\phi(u)$ is a monotonically increasing function with a minimum value of $2/\sqrt{\pi}$ at $u = 0$. A new function $g_2(V,\theta|v)$ which satisfies the inequality (8) can now be defined by replacing $U/u\phi(u)$ by $U\sqrt{\pi}/2$ and $u/u\phi(u)$ by unity, giving

$$g_2(V,\theta|v) \, V^2 dV d(\cos\theta)d\phi = (\frac{\sqrt{\pi}U}{2} + 1) \frac{e^{-U^2} U^2 dU d(\cos\theta)d\phi}{(\pi)^{3/2}} \quad (10)$$

Integration of equation (10) over all space shows that

$$\int_{\text{All space}} g_2(V,\theta|v) \, d^3 \vec{V} = 2 \quad (11)$$

Since g_2 is a function of V only, we can perform the angular integrations and write for the cumulative distribution function

$$\int_0^W g_2(V)V^2 dV = \psi(W) = \frac{4}{\sqrt{\pi}} \int_0^W e^{-U^2}(1 + \frac{\sqrt{\pi}}{2} U) U^2 dU \quad (12)$$

where $\psi(W)$ is defined by equation (12). Now define $W(\xi)$ by the equation

$$\xi = \frac{\xi(W)}{\psi(\infty)} = \int_0^{W(\xi)} e^{-U^2}(\frac{2}{\sqrt{\pi}} + U) U^2 \, dU \quad (13)$$

The procedure for choosing a V and a θ from the distribution function $p(V,\theta|v)$ consists of the following:

- 19 -

(a) Choose a random number ξ_1 in the interval
(0,1) and find the corresponding $W(\xi_1)$. This is done
by consulting a table for $W(\xi)$ which is stored in the
machine. Calculate $\sqrt{\frac{2kT}{M}}\ W(\xi_1)$ and set this equal to V.

(b) Choose random direction angles θ and ϕ ,
thus obtaining the components of V.

(c) Evaluate $p(V,\theta|v)$ and $g_2(V,\theta|v)$.

(d) Choose another random number ξ_2 in (0,1)
and test if

$$\xi_2 g_2(V,\theta|v) \leq p(V,\theta|v) \tag{14}$$

If the inequality holds, accept the velocity V of the
proton and calculate the new velocity of the neutron
assuming that the collision is spherically symmetric in
the center of mass system. If the inequality does not
hold, reject the velocity V, return to (a), and begin
the choosing procedure again. Since the integral over
all space of g_2 is twice that of p, the rejection
rate of V will be one-half. In this way proton
velocities are chosen with the correct distribution,
and the neutron velocities after impact can be found.

Cross-section data are taken from the Brookhaven
compilation [4]. In hydrogen, the constant scattering
cross-section is taken to be 20 barns. The absorption
cross-section in hydrogen is assumed to be strictly

1/V and to have a value of 0.33 barns at room temperature (2200 m/sec.). In the fuel, which consists of ordinary uranium slightly enriched to a little over 1 % U^{235}, the scattering cross-section is assumed to be constant and the same in both isotopes. The absorption cross-section is assumed to be 1/v in U^{238}. The correction to a 1/v cross-section given in BNL-325 [4] for U^{235} is fitted by a quadratic and is included in the absorption cross-section calculation. The degree of enrichment is one of the input parameters and the code actually calculates fuel absorption and scattering cross-sections for the given ratio of U^{235}. As indicated above at a scattering of a neutron by uranium, the former is assumed to emerge with its velocity (and energy) unchanged but with a direction chosen at random from a symmetric distribution.

4. Sampling Procedure

If the straightforward sampling procedure outlined above is used, a tally T is kept of the number of absorptions in fuel and then thermal utilization is obtained by the relation

$$f = \frac{T}{N} \qquad (15)$$

where N is the total number of histories. However, this procedure is very inefficient. In the first place this method inherently has the largest variance of any possible sampling procedure so that many histories must be processed in order to get a good estimate of f. Secondly, in each history only the very last collision is of any interest, and in many cases scores or even a few hundred collisions must be followed before the neutron is finally absorbed. It therefore seemed advantageous to start off each history with a weight $w_0 = 1$, say, and at each collision in fuel reduce the weight by the fraction $\sum_a^{(F)}/(\sum_a^{(F)} + \sum_s^{(F)})$ where $\sum_a^{(F)}$ and $\sum_s^{(F)}$ are the macroscopic cross-sections for absorption and scattering respectively. By this procedure it was hoped to obtain for each history a fair estimate for f thus reducing the variance. Scatterings in the moderator were treated as in the straightforward method. The results using this weighting

technique were disappointing. It was found that for
most histories the weight when the neutron was absorbed
in moderator was either 1 or else close to zero; that
is, either a neutron was absorbed before entering the
fuel or else it suffered several collisions in the fuel
with the result that its weight was reduced to a very
small fraction. Thus neither of the disadvantages of
the straightforward sampling procedure were much
improved upon. The variance was reduced slightly but
the number of scattering collisions per history was
increased since now there were no terminations in the
fuel. It is clear that the roles of fuel and moderator
could have been interchanged i.e. reduce the weight by
the appropriate factor at moderator collisions and
terminate by the straightforward sampling technique at
fuel collisions, but this did not offer any prospect
of a real improvement in efficiency. The obvious
procedure is to reduce the weight at collisions in both
the moderator and fuel, tallying the deposition of the
weight in one medium or the other. This would have the
advantage that data would be obtained from each and
every collision; however, there is the fatal drawback
that the first history would never terminate -- the
neutron would continue on its path forever and its weight
would soon be reduced to a value $< 10^{-11}$, the smallest

UNIVAC number. One possible method would be reduce the
weight at collisions in both media and to terminate
histories arbitrarily once the weight were reduced to
some very small number, say 10^{-3}. However, this is
not a statistically justifiable procedure, and further-
more since it takes twice as many collisions on the
average to reduce the weight from 10^{-1} to 10^{-3} as
from 10^{0} to 10^{-1}, two-thirds of the computing time
is taken up in adding a very little correction to the
data, for by the time the weight is reduced to 10^{-1},
nine-tenths of the weight has been deposited in one
medium or the other and a lot of computing time is
taken up in depositing most of the remaining 10 %.

A much better method of terminating histories is
to play a game of Russian roulette once the weight is
first reduced below some pre-assigned value W_c. After
each collision the weight is examined to determine if
it is less than the cut-off value W_c. If not the
history continues, but once the weight is found to be
less than W_c a random number ξ is chosen. If
$\xi > W_c$ the history is terminated and two numbers are
tallied, the amount of weight W_F deposited in the
fuel, and the amount W_M deposited in the moderator.
If $\xi \leq W_c$, then the history is continued from the
point where the last collision took place but the

weight increased by multiplying it by $1/W_c$. When
the weight is reduced again below W_c Russian roulette
is played once more. For histories which are regenerated
(and a history will be regenerated n times with proba-
bility $(W_c)^n$) the tallies are made of the total amount
of weight deposited in each medium and it is clear that
individual tallies can exceed unity. To simplify the
coding, this procedure is altered somewhat. Once the
weight is reduced below W_c, a random number is chosen
and tested against the actual weight W. If $\xi > W$ the
history is terminated and the tallies made. If $\xi \leq W$
the weight is increased to unity and the history is
continued. The probability of regeneration is some-
what reduced since $W < W_c$ when the test is made, but
the two methods are both statistically correct.

Now the thermal utilization factor is estimated
by evaluating the ratio $W_F/(W_F+W_M)$ for each history
and averaging over all histories. Notice that (W_F+W_M)
is the total weight deposited and the sum of this
quantity over all histories should equal, on the
average, the total number of histories processed.

The results using this sampling procedure give a
startling improvement over the simple method tried first.
Defining efficiency of a sampling procedure as the time
required to achieve some predetermined probable error,

the Russian roulette sampling technique is about sixteen
times more efficient than the first one described in
this section. It was found that on the average only
one-fourth as many collisions per history had to be
calculated and that the variance was reduced by about
one-half (giving a reduction of one-quarter when the
square-root is taken in calculating the probable error).
To some extent the efficiency obtained depends upon the
value chosen for the cut-off weight W_c. On the one
hand a large W_c requires the processing of only a
few collisions per history, but on the other, a large
W_c gives rise to a large variance. A small test
problem was run on the UNIVAC to see if W_c could be
optimized. In this test, neutrons were assigned, at
each collision, probabilities of remaining in the same
medium or going into the other. At each collision the
weight was reduced by a constant factor in each medium.
Thus all the geometry and scattering calculations were
eliminated for the test purposes. The results showed
that the best value for W_c was unity, i.e. Russian
roulette should be played at every collision. The
efficiency decreased slowly until W_c was of the order
of one-tenth when the decrease became quite rapid.
Short tests run with the actual code indicated a rather
broad minimum in efficiency in the range $0.4 < W_c < 0.75$.

The reason $W_c = 1$ is somewhat less efficient than
a lower value is that it takes the machine a certain
amount of time to make the tallies at the end of each
history and also some time to begin a history, whereas
in the test codes these times were extremely short.
Using $W_c = 1/2$, about 200 to 250 histories per hour
are processed for the lattices used. A probable error
of 1 % is obtained for about 100 histories.

5. Results

In Table I results obtained for three different lattices are shown. As already explained, the lattices used were matched to some of those in WAPD 151 [1] and data in the first four columns are selected from this report. Results presented here were obtained by processing about 400 histories, which required close to two hours machine computation in each case.

Table I

$\frac{W}{U}$ Volume	Fuel Rod Diameter (inches)	Enrichment % U^{235}	Thermal Utilization	
			WAPD-151	UNIVAC Code
2	.600	1.158	.881 ± .004	.883 ± .004
3	.387	1.311	.857 ± .004	.885 ± .004
2	.387	1.311	.904 ± .003	.906 ± .003

In addition to the thermal utilization some data were collected on the distributions both in energy and in space of the scatterings. For such a small number of histories not very good statistics can be obtained, but the energy distribution both in moderator and fuel seemed to show a Maxwell-Boltzmann distribution with a high energy tail. Since, on the average there were

only about two scatterings per history in the fuel, it
was not possible to ascertain if there was any appreci-
able hardening of the spectrum in fuel. Also statistics
were taken of the energy distribution of neutrons enter-
ing the fuel. Data again were too sparse to draw any
conclusions except that the spectrum seemed to be very
similar to that in the moderator. As far as spatial
distribution was concerned, the fuel rod was divided
into two regions of equal area, an inner region and
an outer one. Scatterings seemed to take place equally
in both regions -- there was no discernable increase in
outer region as was expected. It should be emphasized
though that the effect is probably small and may have been
masked by statistical error. Furthermore all scatterings
were weighted equally whereas in fact neutrons undergoing
scattering had weights ranging from one to 1/2, and this
is true of the energy spectrum data also.

6. Discussion

The results presented in the previous section show that a Monte Carlo procedure is capable of giving a good estimate of thermal utilization. However, in view of the simplifications made in writing this code it is not expected that accurate results can be obtained with it. It should be emphasized that the probable errors quoted in the last column in Table I are those due to the statistical nature of the calculation whereas the errors given for the experimental results are those due to uncertainty in certain measurements and the two are in no way related. By increasing the number of histories, or improving the sampling technique, the probable error obtained in a Monte Carlo calculation could be reduced, but there would still remain those errors due to approximations made in the calculations as well as those due to inaccurate data. It is possible to evaluate the effect of changing, say, the hydrogen scattering cross-section by a few percent by making this change and running the problem again. There are several factors viz. all the cross-section data and the starting-off distribution which inherently have some uncertainty attached to them, and estimation of an overall error in f due to these uncertainties is difficult. However, this is a difficulty which is

present in any attempt to calculate f by any method
whatsoever.

In view of the approximations and simplifications
made the excellent agreement with experiment shown in
Table I must be regarded as somewhat fortuitous. To
expand the UNIVAC code to take into account collisions
in the aluminum cladding and in the oxygen in the
moderator, as well as improving model of the water
molecule would be possible, but such a code would be
greater than one memory load and the use of tape
storage would increase the running time beyond all
practicality. The advent of the IBM-704 does make
this expanded code a practical project and work on
such a code has already begun. This code will treat
a hexagonal lattice, it will be capable of treating
atoms other than hydrogen and uranium and collisions
with these atoms will take recoil into account.
Furthermore work is progressing on a much more sophisti-
cated model of the water molecule which will take into
account the effects of inelastic scatterings by using
a quantum-mechanical isotropic oscillator model for
the molecule.

Consideration has been given to the possibility of
calculating thermal utilization for graphite moderated
reactors. Since crystal effects in graphite come into

play only for energies much below thermal it seems that
inelastic collisions in graphite can be ignored. However,
work done elsewhere [5] indicates that such a calculation
would be extremely time consuming since a thermal neutron
in graphite might make several hundred collisions before
entering the fuel. A technique widely used in doing
shielding calculations by Monte Carlo might be adapted
profitably in this case. If the model of cylindrical
fuel rods embedded in the moderator in a lattice arrange-
ment is retained, several imaginary cylindrical surfaces
concentric with the fuel rod are considered. These
"doubling" surfaces would be of the order of a mean free
path apart and a neutron crossing such a surface would be
subjected to a sort of Russian roulette. A neutron that
is travelling away from the fuel would survive the game
with probability $1/p$ say and continue with weight
increased by a factor p. A neutron travelling in towards
the fuel rod would have its weight reduced by $1/p$ but p
identical neutrons would be continued from the point of
crossing the doubling surface. In this way the more
important neutrons would be followed in detail and little
time wasted in following those buried deep in the graphite.
Another possibility is to assume that diffusion theory
holds after a distance of one mean free path inside the
moderator and do the Monte Carlo calculation only in the
fuel rod and its immediate surroundings.

BIBLIOGRAPHY

[1] Kranz, A. Z. and Smith, G. G., <u>A Second Report of
     Measurements of f, p and ε of Water Moderated
     Slightly Enriched Uranium Lattices</u>. WAPD-151
     (May 1956).

[2] von Neumann, J., <u>Various Techniques Used in
     Connection with Random Digits</u>. National Bureau
     of Standards, AMS12 (1951), p. 36.

[3] Wigner, E. P. and Wilkins, Jr., J. E., <u>Effect of
     the Temperature of the Moderator on the Velocity
     Distribution of Neutrons with Numerical Calcula-
     tions for H as Moderator</u>. AECD-2275 (Sept.
     1944).

[4] Hughes, D. J. and Harvey, J. A., <u>Neutron Cross
     Sections</u>, BNL 325 (July 1955).

[5] Sampson, J. B., <u>Attempted Monte Carlo Calculation
     of Resonance Escape Probability in a Graphite
     Lattice</u>. Proceedings of the Brookhaven Conference
     on Resonance Absorption of Neutrons in Nuclear
     Reactors (BNL 433) (Sept. 1956), p. 92.

Date Due